Combustion Research Facility PUS



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Pool fire and fuel film imaging in a spark ignition engine

More than 60 percent of the unburned hydrocarbon (UHC) emissions measured during the federal test procedure for a port fuel-injected spark-ignition engine are collected in the first two minutes, when the engine and catalyst are cold. During this period, it is known that liquid films form on the walls of the intake port and combustion chamber, making it extremely difficult to manage fuel injection duration during a cold start.

Pete Witze and Duane Sunnarborg have spent the last two years designing and assembling a new optical engine facility to study this problem. The single-cylinder engine consists of a 1994 production four-valve head mounted on a quick-release, dropdown cylinder mechanism designed by Duane. The hydraulically supported cylinder can be lowered approximately 10 cm in less than one minute, to allow cleaning of the window in the piston crown and rapid reassembly.

Pete has developed an asynchronous reset capability that permits the use of a conventional color video camera to record synchronous images of the combustion event with 100 µs exposure duration. He has observed that fuel films on the combustion chamber walls burn as diffusion-controlled pool fires, emitting bright, visible emissions during the expansion stroke as shown in the figure (a). In addition to UHC emissions associated with these rich flames, it is also believed that the liquid films seen burning near the exhaust valves escape the combustion chamber during the exhaust stroke.

While these pool fires serve as a useful marker of liquid films, the

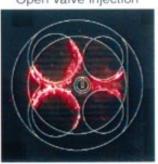
technique only works if the films are burning, which often is not the case during a cold start. To observe these liquid fuel films directly, Bob Green developed a flood-illuminated laser-induced fluorescence (LIF) imaging technique. A diverging Nd:YAG laser beam at 355 nm is used to illuminate the combustion chamber through the piston. Fluorescence at 450 nm from regular gasoline is recorded with an intensified CCD camera through a narrow bandpass filter.

The LIF images shown in the figure (b) are similar in pattern to the pool fire images, and are observed in all portions of the cold start test sequence

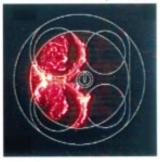
where liquid fuel films are present. In contrast, the wall films marked by the pool fires are only observed during the expansion stroke of cycles that burn hotly enough to ignite the liquid fuel.

These imaging techniques, together with other diagnostic tools, are being used to evaluate different fuel-injector designs and strategies as part of a project funded by the DOE Office of Transportation Technologies through a CRADA with the Low Emission Partnership of the U.S. Council for Automotive Research (USCAR), as part of the Partnership for a New Generation of Vehicles (PNGV).

Open valve injection



Closed valve injection



(a) Pool fire emissions





(b) Laser-induced fluorescence

In-cylinder images of visible emissions from pool fires (a) and laser-induced fluorescence from fuel films (b), comparing open and closed valve injection for the 15th engine cycle of a simulated cold start. The larger intake valves are on the left-hand side of each picture. The concentric circles indicate the cylinder bore and clear aperture through the window in the piston.

Ultra-low NO_x burner tested in the BERL

An ultra-low NO_x burner designed to fire natural gas and refinery fuel gas in process heaters for the petroleum industry was recently tested in the Burner Engineering Research Lab (BERL) by Neal Fornaciari, Peter Walsh, Lloyd Claytor, and Philippe Goix with Peter Loftus and Roberto Pellizzari of Arthur D. Little (ADL) of Cambridge, Massachusetts. The purpose of the trials was to perform a detailed study of the prototype low emissions burner flame, to provide data for model verification, and to identify potential design improvements.

The development of the burner is supported by the Gas Research Institute (GRI) under a program managed by Richard Petrich, and the burner design is the product of collaboration between Peter Loftus, Charles Benson, and Roberto Pellizzari of ADL and Richard Martin of Callidus Technologies of Tulsa, Oklahoma.

The appearance of the flame from the ADL/Callidus burner through the windows of the BERL furnace is shown in Figure 1. During the tests of the burner at its full firing rate and 15% excess air, there were only eight parts per million of the air-polluting nitrogen oxides, NO and $\mathrm{NO_2}$ ($\mathrm{NO_x}$), in the combustion products. The burner was operated successfully on both natural gas and simulated refinery gas.

Mie scattering images obtained by Philippe are shown in Figure 2. The images were produced by illuminating the region just above the burner exit (the region visible through the bottom window in Figure 1) with a sheet of laser light, shortly after introducing titanium dioxide particles into the combustion air.

In the top part of Figure 2 the brightest regions are relatively cold, unmixed, unreacted air. The less bright region in the center of the image contains hot, well-mixed combustion products. The instantaneous location of the flame, not visible because its emission is much weaker than the laser, is at the highly irregular boundary between the two regions. At one-third of full load, the lower image in Figure 2 shows that the central region is less well mixed and that unreacted air is distributed throughout the flow.

The data from BERL provided the development team with an understanding of how the combustion process is effective in achieving very low emissions while also providing a high degree of flame stability. The data will also serve to calibrate analytical models used in developing the prototype design and will be helpful in scaling up the burner. The ADL/Callidus team will incorporate knowledge gained from the BERL trials into an industrial version of the burner. expected to be on the market in 1997, providing lower emissions than required by any current or foreseen environmental regulation.

The BERL facility is supported by GRI under a program managed by Robert Gemmer and by the U.S. Department of Energy, Office of Industrial Technologies, under the direction of Gideon Varga.



Figure 1. 530 kW natural gas flame from the ADL/Callidus burner seen through the windows of the furnace in the Burner Engineering Research Lab.

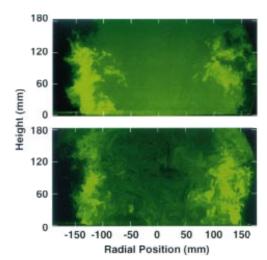


Figure 2. Mie scattering images obtained after introducing titanium dioxide particles into the combustion air and illuminating the flow with a narrow sheet of laser radiation. Top: at full firing rate of 530 kW. Bottom: at 176 kW. Mixing of air with fuel and combustion products is slower at the lower firing rate.

Combustion Research Facility Phase II Workshop

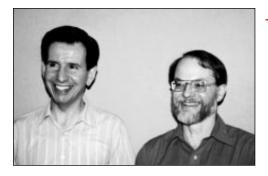
Funds have been authorized for completion of the Phase II addition to the Combustion Research Facility. The project will increase our office space from 25,000 to 36,000 sq. ft. and our laboratory space from 16,400 to 37,600 sq. ft.

A workshop was held June 13-14, 1996 to solicit user input on the research capabilities that should be emphasized in this addition. Attendees included members of both the university and industrial combustion research communities as well as representatives from a number of interested government organizations.

After a series of overview presentations by CRF management on current capabilities and possible new or expanded directions a set of six working groups, each chaired by a member of the external research community, was convened to develop recommendations in the areas of diagnostics, modeling and simulation, high-pressure combustion, combustion chemistry, industrial processes, and new programs. The workshop culminated in a series of recommendations from each of these sub groups.

As might be expected, the suggestions offered exceeded the available budget. During the next couple of months, CRF management working closely with our DOE Basic Energy Sciences sponsor, will use the results of the workshop and additional input from the external community to finalize the Phase II definition.

It is expected that construction will begin on the office addition in the summer of 1996 and that laboratory construction will begin in 1997.

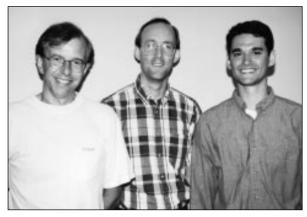


Adams and Bastress Awards

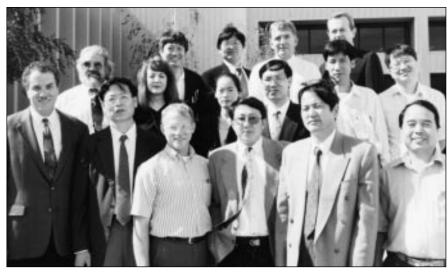
The annual presentation of these two prestigious Sandia awards was made in June to Alan Kerstein (left) and John Dec (right), respectively.

The O.W. Adams Award was given to Alan with the following citation: "Alan has made outstanding contributions to CRF research programs in modeling studies of spray, coal, and turbulent combustion. Alan's extraordinary breadth, creativity, and clarity of expression have led to many valuable collaborations, both internal and external to Sandia."

John's E. K. Bastress Award reads: "John has redefined the understanding of in-cylinder soot formation processes for the diesel engine community. Through his direct link with Cummins and his active participation in the SAE, John has successfully transferred this new insight to effect change in engine design."



Dr. Francis Teyssandier (left) of CNRS in Perpignon, France, is nearing the end of a one-year sabbatical with Mark Allendorf (center). Francis and Mark are using computational methods to predict rates of chemical reactions occurring in high-temperature materials synthesis processes. Tom Arsenlis (right), a Cornell Co-op student working with Mark, helped construct and test a new stagnation-flow reactor, and is now using it to investigate the formation of titanium nitride films using chemical vapor deposition methods.



A workshop on Atmospheric Sciences and Non-Proliferation was held in Livermore in June. CRF Director Bill McLean (front row, left) hosted a tour of the CRF for the Chinese delegation, headed by Dr. Peng Hansheng, Associate Director of the Chinese Academy of Engineering Physics and Chairman of the Chinese Steering committee (front row, next to Bill).



Winners from the Combustion Research Facility of the 1996 Sandia National Laboratories' Employee Recognition Awards (from left to right): Herb Blair, Technical Excellence; Dave Chandler, Teamwork; Jay Keller, Leadership; and Dave Rakestraw, Leadership. The annual awards, given by Lockheed Martin, honor individuals and teams for outstanding service to Sandia and the nation.

Dec winner of Horning Award

Once again the prestigious Society of Automotive Engineers (SAE) Horning Award comes to the CRF. John Dec (pictured) and Christoph Espey, now of Daimler-Benz, Germany, have jointly won for a paper they wrote entitled, "Ignition and Early Soot Formation in a DI Diesel Engine Using Multiple 2-D Imaging Diagnostics" (SAE Paper No. 950456). The award will be presented October 16 during the 1996 SAE Fuels & Lubricants Meeting in San Antonio, Texas.

Previous winners of the Horning Award from the CRF include T. Michal Dyer (1979) and Pete Witze (1985).



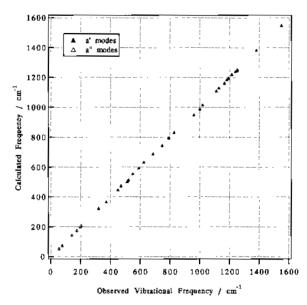
Experiment and Theory Characterize Benzo[a]pyrene Transition

Concerns over air toxics have stimulated efforts by Eric Rohlfing, post-doc Chris Gittins, and Celeste Rohlfing to identify and quantify trace by-products resulting from the incomplete combustion of hydrocarbon fuels. Polycyclic aromatic hydrocarbons (PAHs) are of particular concern because of their adverse biological effects and their role in the formation of soot.

At present, PAH emissions are quantified by sampling a large amount of burner exhaust, and analysis is not completed for weeks after the sample is taken. Thus the current method of analysis does not provide the real-time feedback necessary to actively control emissions.

Current research by the CRF team is aimed at developing a simple on-line method for quantifying PAH emissions using isomer-selective resonanceenhanced multiphoton-ionization time-of-flight/mass spectroscopy (REMPI-TOF/MS). The combination of mass and wavelength discrimination makes REMPI/TOF-MS a powerful technique for identification of individual species in a multicomponent mixture. The ability to distinguish between isomers is also essential from a regulatory standpoint because one isomer may be extremely hazardous while the other is relatively benign, e.g., benzo[a]pyrene (BAP) vs. perylene.

The initial CRF efforts to develop REMPI/TOF-MS as an on-line diagnostic required confirmation of BAP spectroscopy for validation of the proposed scheme. It was essential to employ high-accuracy quantum chemical calculations of the first excited state of BAP in order to assign the observed spectral features. A total of 27 modes of a' symmetry and 5 of a" symmetry were unambiguously identified. The figure illustrates the excellent agreement between the calculated vibrational frequencies and those observed experimentally for the first excited state of BAP. 🤌



Calculated vibrational modes for the first excited state of BAP are used in making unique assignments of those measured experimentally.

CRF home page

The Combustion Research Facility has a site on the Worldwide Web at http://www.ca.sandia.gov/CRF/. Certain elements are under construction and additions will be made along the way. We would appreciate your comments.

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